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ROLE OF THE POLARIZATION EFFECTS AT INELASTIC
COLLISIONS OF ELECTRONS WITH ATOMS [   ]

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$$k\,\mathrm{ctg}\,\delta(k) = -\frac{1}{a} + \frac{1}{2}r_0 k^2 + \cdots ,$$

valid for short-range forces, is superseded by another expansion:

$$k\,\mathrm{ctg}\,\delta(k) = -\frac{1}{a} + \frac{\pi \alpha k}{3a^2} + \frac{4\alpha k^2}{3a}\ln\,(1,23k\sqrt{\alpha}) + 0(k^2).$$

It is natural to expect that the polarization of the atom exerts a substantial effect on excitation functions near the threshold, when, upon collision, the electron has a low velocity.

Equations for inelastic collisions are formulated in the present work, taking into account the virtual transitions that include the standard system of equations brought up in the book [3] as a particular case. In order to find the obvious form of polarization potentials in the adiabatic approximation, it is proposed to utilise the corresponding variational principle. As a matter of example a simple rated formula is brought up, which was obtained by the variation of one parameter. Then the dependence of excitation cross section on energy near the threshold is being investigated.

1. DERIVING THE EQUATIONS.

Scattering in the system "electron + atom" is described by the equation

$$(H_0(r) - T_R + W(rR) - E)\Psi(rR) = (H-E)\Psi(rR) = 0, \quad (1)$$

where r is the aggregate of radii-vectors of atomic electrons, R is the radius-vector of the incident electron,

$$T_R = \frac{1}{2}\Delta_R^2,$$

$W(rR) = -\frac{1}{R} + \sum_{i=1}^{z}\frac{1}{|r_i - R|}$ is the interaction energy of the electron with the atom, E is the total energy of the system.

We shall expand $\Psi(rR)$ by the system of eigenfunctions $\Phi_n(r)$, belonging to atom's energetic levels ε_n:

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INTRODUCTION

A substantial role of polarization effects arising at
inelastic collisions of electrons and atoms has been lately ascer-
tained. It has resulted that the influence of polarization is
particularly manifest at low energies.

There are two basic methods of accounting for atom polari-
zation. One of them consists in accounting the virtual transitions
into excited atomic states. The influence of virtual transitions in
the adiabatic approximation is equivalent to the action of the com-
plementary polarization potential having at great distances r the
form — $\alpha/2r^4$, where α is the polarizability of the atom. The
other method takes into account the distortion of electron density
in the atom by the incident electrons and is called "method of pola-
rized orbits" [1]. The accounting of polarization changes the nume-
rical value of distance length as well as the character of phase
dependence on energy. It was shown in particular [2] that the well
known expansion

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* (ROL' POLYARIZATSIONNYKH EFFEKTOV PRI NEUPRUGIKH STOLKNOVENIYAKH
ELEKTRONOV S ATOMAMI)

$$\Psi(rR) = \sum_{n=1}^{\infty} F_n(R)\Phi_n(r). \tag{2}$$

From the steady-state condition of the functional $\int \Psi(rR)(H-E)\Psi'(rR)\,d\tau$ at $F_n(R)$ variation we shall obtain the following system of equations :

$$\left(T_R + \frac{k_n^2}{2}\right)F_n = L_n F_n = \sum_{m=1}^{\infty} V_{nm}F_m. \tag{3}$$

Here

$$\frac{k_n^2}{2} = E - \varepsilon_n; \quad V_{nm} = \int \Phi_n W \Phi_m \, dr.$$

Let us consider first of all the case when the energy of incident particles is sufficient for exciting the first levels which are considered tightly bound with one another, but not with the fundamental level.

The usual consideration amounts to the solution of the finite system

$$L_n F_n = \sum_{m=1}^{N} V_{nm}F_m \quad (n=1 \ldots N) \tag{4}$$

with either subsequent approximations. The functions F_n have an asymptotic form :

$$F_n \sim e^{ik_nR}\delta_{1n} + f_n(\vartheta, \varphi)\frac{e^{ik_nR}}{R} \quad (R \to \infty).$$

Let us set up the problem of accounting to a specific extent the effect of closed reaction channels upon the open ones, i.e. the effect of virtual transitions onto the levels $N + 1$, $N + 2 \ldots$

It is currently well known from the theory of elastic collisions that the accounting of virtual interaction with excited states changes significantly the pattern of scattering (see for example the expressions of [4]). From equations (3) we have

$$L_1 F_1 = \sum_{\alpha=1}^{\infty} V_{1\alpha} F_\alpha;$$

$$L_n F_n = \sum_{\beta=1}^{N} V_{n\beta}F_\beta + \sum_{\gamma>N} V_{n\gamma}F_\gamma; \quad (n=2 \ldots N); \tag{5}$$

$$L_\gamma F_\gamma = \sum_{\gamma'=1}^{\infty} V_{\gamma\gamma'} F_{\gamma'}.$$

In the last equation we assume approximately

$$L_\gamma F_\gamma \approx V_{\gamma 1} F_1 + \sum_{n=2}^{N} V_{\gamma n} F_n. \qquad (6)$$

This approximation is equivalent to a complementary accounting of virtual bindings of γ levels with the basic one and with the group N of closely bound levels.

Expressing F_γ in the form

$$F_\gamma = L_\gamma^{-1} \left[V_{\gamma 1} F_1 + \sum_{n=2}^{N} V_{\gamma n} F_n \right], \qquad (6a)$$

we obtain the following system of equations :

$$\left(L_1 - V_{11} - \sum_{\alpha \neq 1}^{\infty} V_{1\alpha} L_\alpha^{-1} V_{\alpha 1} \right) F_1 = L_1 F_1 = 0, \qquad (7)$$

$$L_n F_n = \sum_{\beta=1}^{N} U_{n\beta} F_\beta \quad (n = 2 \ldots N), \qquad (8)$$

where $\quad U_{n\beta} = V_{n\beta} + \sum_{\gamma > N} V_{n\gamma} L_\gamma^{-1} V_{\gamma\beta}.$

At $N \to \infty$ this system passes to equations (3), and for any finite N it contains the system (4) as a particular case (see also [5]).

From the system (7 – 8) follow in particular approximations of tight bond and distorted waves, taking into account the polarization. N represents a generalization of the corresponding method with accounting of polarization precisely in the case of tight bond of two or more levels of the system of equations (8) with n = 1 ....
Physically the situation considered is for example materialized at 3S — 3P excitation in the Na atom, 2S — 2P — in the H atom, and so forth.

In another boundary case, when a group of tightly bound levels is reduced to a single one, we obtain the method of distorted waves with the accounting of polarization for the transition 1 — n:

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$$L_1 F_1 = 0;$$
$$L_n F_n = U_{n1} F_1 + U_{nn} F_n \qquad (9)$$

with

$$U_{nk} = V_{nk} + \sum_{\gamma \neq 1, \neq n} V_{n\gamma} L_{\gamma}^{-1} V_{\gamma k} \qquad (k = 1, n).$$

With the view of summing up approximately the expressions for the potentials, we transform the equations (7 - 8) as follows:

$$L_1 F_1 = 0;$$
$$L_n F_n = \sum_{m=1(\neq n)}^{N} V_{nm}^{p} F_m + \sum_{m=1(\neq n)}^{N} V_{nm} \left[F_m - \sum_{p=1(\neq m)}^{N} L_m^{-1} V_{mp} F_p \right] - \\ - V_{nn} L_n^{-1} \sum_{m=1(\neq n)}^{N} V_{nm} F_m. \qquad (8a)$$

Here

$$V_{nm}^{p} = \sum_{\alpha \neq m}^{\infty} V_{n\alpha} L_{\alpha}^{-1} V_{\alpha m}. \qquad (10)$$

The designation L_n is obvious from the equation (7).

At the same time the system (9) has the form:

$$L_1 F_1 = 0;$$
$$L_n F_n = V_{n1}^{p} F_1 + V_{n1}[F_1 - L_1^{-1} V_{1n} F_n] - V_{nn} L_n^{-1} V_{n1} F_1. \qquad (9a)$$

The potentials, represented in the obtained equations by sums, account to a well known measure the interaction between excited states and are called polarization potentials. The latter are nonlocal operators, as may be seen from the expression (10). Thus, for the factual summing up, the so-called adiabatic approximation must be introduced, and in which the kinetic energy operator is substituted by a number. Let us remark that this approximation is only valid at great distances.

The method of computation of polarization potentials is analyzed at further length in the next section.

2. COMPUTATION OF POLARIZATION POTENTIALS.

We shall show that

$$V_{nm}^{p} F_m = \sum_{\alpha \neq m}^{\infty} V_{n\alpha} L_{\alpha}^{-1} V_{\alpha m} F_m = \int \Phi_n W g_m \, dr F_{nn} \qquad (11)$$

where $g_m(rR)F_m(R)$ satisfies the equation

$$(H_0(r)-T_R-E)g_mF_m=[V_{mm}(R)-W(rR)]\Phi_m(r)F_m(R). \quad (12)$$

In reality,

$$g_mF_m=\sum_{\alpha\neq m}^{\infty}\Phi_\alpha(T_R+E-\varepsilon_\alpha)^{-1}V_{\alpha m}F_{m}=\sum_{\alpha\neq m}^{\infty}\Phi_\alpha L_\alpha^{-1}V_{\alpha m}F_{m}, \quad (13)$$

and, substituting this into the equation (11), we shall obtain the left-hand part. The investigation of the equation (12) constitutes an independent problem. But for our objectives it will be subsequently sufficient to limit ourselves to the adiabatic approximation, in which the equation (12) passes into

$$(H_0(r)-\varepsilon_m)g_m^{(a)}=(V_{mm}-W)\Phi_m. \quad (14)$$

As is shown in reference [6], the functions $g_m^{(a)}$ can be practically computed by the variational method using the functional

$$I_m[g_m^{(a)}]=\int g_m^{(a)}\{(H_0-\varepsilon_m)g_m^{(a)}+2W\Phi_m\}\,dr. \quad (15)$$

At the same time

$$\min I_m[g_m^{(a)}]=V_{mm}^p(R). \quad (16)$$

At $m=1$ (basic state) V_{11}^p is found for certain atoms (see for example the works [6, 7]. For the computation of V_{nn}^p at $m=n\neq1$ (excited states) we shall make use of the functional (15).

Taking into account the conditions satisfied by the exact function $g_m^{(a)}$,

$$\int\Phi_n(r)g_n^{(a)}(rR)\,dr=0;$$

$$\int\Phi_k(r)g_n^{(a)}(rR)\,dr=\frac{V_{nk}}{\varepsilon_n-\varepsilon_k} \quad (k=1\ldots n-1), \quad (17)$$

we shall admit that

$$g_n^{(a)}=(t-\bar{t})\Phi_n+\sum_{k=1}^{n-1}C_{nk}\Phi_k; \quad (18)$$

$$C_{nk}=\frac{V_{nk}}{\varepsilon_n-\varepsilon_k}-t_{nk}$$

(see also the work [8]), where t is an arbitrary function from parameters, the stroke denoting the averaging by the state Φ_n.

It is obvious that the possible exact solution of the equation (14) does not imply the maximum approximation to the exact potential, particularly in the vicinity of atom boundaries. It is thus desirable to choose t in a form which would allow foregoing complex computations in a region where the adiabatic approximation is definitely unreal, and would lead to a good asymptotic behavior. Limiting ourselves to a single parameter, we shall estimate that

$$ t = \begin{cases} aW_1 = a\dfrac{r}{R^2}P_1(\cos\theta) = a\dfrac{z}{R^2} & (R>r) \\[2mm] 0 & (R\leqslant r) \end{cases} \qquad (19) $$

(at the same time if $R \leqslant r$; $C_{n_k} = 0$; we denote by W_1 the longest-acting, dipole part of energy of the perturbation W).

With the function (18), the functional I_n is:

$$ I_n = 2\left[(t-\bar{t})W_1 + \tfrac{1}{4}(\Delta t)^2\right]_{nn} + $$

$$ + 2\sum_{k=1}^{n-1} C_{nk}[(\varepsilon_k-\varepsilon_n)t + W_1]_{nk} + \sum_{k=1}^{n-1} C_{nk}^2(\varepsilon_n-\varepsilon_k). \qquad (20) $$

Substituting here the formula (19) and varying a(R), we obtain

$$ a(R) = -2\,\frac{\overline{Z^2(R)} - (\overline{Z(R)})^2 - \sum_{k=1}^{n-1} Z_{nk}^2(R)}{1 - 2\sum_{k=1}^{n-1} Z_{nk}^2(R)[\varepsilon_k-\varepsilon_n]}. \qquad (21) $$

Then, the diagonal polarization potential will be

$$ V_{nn}^p(R) = \frac{1}{R^4}\left\{a^2\left[\frac{1}{2} - \sum_{k=1}^{n-1} Z_{nk}(\varepsilon_k-\varepsilon_n)\right] + \right. $$

$$ \left. + 2a\left[\bar{Z}^2 - (\bar{Z})^2 - \sum_{k=1}^{n-1} Z_{nk}^2\right] - \sum_{k=1}^{n-1} Z_{nk}^2/.\varepsilon_k - \varepsilon_n\right\} = -\frac{\alpha_n(R)}{2R^4}. \qquad (22) $$

Here $Z_{nk} = \int_0^R \Phi_n W \Phi_k\, dr$ and so forth

At $R \to \infty$ V_{nn}^p passes into $-\alpha_n(\infty)/2R^4$ with a polarizability

$$\alpha_n(\infty) = \frac{4\overline{Z^2(\infty)} - (\overline{Z(\infty)})^2 - \sum_{nk} Z_{nk}^2(\infty)}{1 - 2\Sigma_k Z_{nk}^2(\infty)(\varepsilon_k - \varepsilon_n)} - 2\sum_k \frac{Z_{nk}^2(\infty)}{(\varepsilon_k - \varepsilon_n)}, \quad (23)$$

which may be directly compared with the experimental value.

Thus, formula (22) allows the finding of an approximate polarization V_{nn}^p potential for any level n, by computing the matrix elements, and not by solving each time the corresponding equation. In the aggregate, the thus found V_{nn}^p is in its absolute value everywhere smaller than the exact adiabatic potential. The nondiagonal matrix elements are found by the formula $V_{mn}^p = \int \Phi_n W g_m^{(a)} dr$ with the extreme functions $g_m^{(a)}(rR)$. Therefore, all the potentials in the equations (7) and (8a) are so determined.

3. DEPENDENCE OF EXCITATION CROSS SECTION ON ENERGY.

Setting up the dependence of the excitation amplitude on the energy k_n^2 of the scattered particles, we shall limit ourselves to the consideration of spherically-symmetrical S - scattering in the case of equation's loose bound (see equation (9a)). At the same time

$$F_1 = \frac{1}{r}, F_n = \frac{\tilde{\varphi}}{r} \quad (24)$$

(in this section r is the radius-vector of the outer electron). Then the system (9a) will pass to

$$f'' + (k_1^2 - \mathcal{V}_{11})f = 0, \quad (25)$$
$$\varphi'' + (k_n^2 - \mathcal{V}_{nn})\tilde{\varphi} = \mathcal{V}_{n1}f, \quad (26)$$

where $\mathcal{V}$ are the full potentials

$$f \to \frac{1}{k_1} \sin k_1 r + q_1 \exp(ik_1 r),$$

$$\tilde{\varphi} \to q_n \exp(ik_n r) \quad r \to \infty \quad (27)$$

The excitation amplitude is $q_n = -\exp(i\tilde{\delta})\int \varphi(r)\,\mathcal{V}_{nl}(r)f(r)\,dr$, where $\varphi(r)$ is the solution of the homogenous equation (26) with the asymptotic $\varphi \to \dfrac{c}{k_n}\sin(k_n r + \tilde{\delta})$.

The equation

$$\varphi'' + (k_n^2 - 2V_{nn} - 2V_{nn}^p)\varphi = 0$$

passes at r greater than a certain R into the equation

$$\varphi'' + (k_n^2 - 2V_{nn}^p)\varphi = 0. \qquad (28)$$

Using the first iteration for the integral representation of φ, we shall obtain

$$\varphi = \frac{1}{k_n}\sin(k_n r + \delta) - \sin(k_n r + \delta)N_1(r) +$$

$$+ \cos(k_n r + \delta)N_2(r). \qquad (29)$$

Here

$$N_1(r) = \frac{1}{2k_n^2}\int_R^r \frac{\sin 2(k_n s + \delta)}{s^4}a_n(s)\,ds, \qquad (30)$$

$$N_2(r) = \frac{1}{k_n^2}\int_R^r \frac{\sin^2(k_n s + \delta)}{s^4}a_n(s)\,ds. \qquad (31)$$

Considering R sufficiently great, so that at $r > R$ $\alpha_n(r) \approx \alpha_n(\infty)$, we obtain

$$N_1(r) = \frac{\alpha_n}{k_n}\left[\frac{2a(R)-3r}{3r^3} - \frac{2a(R)-3R}{3R^3}\right] +$$

$$+ O(k_n \ln k_n) = \frac{Q(r)}{k_n} + O(k_n \ln k_n). \qquad (32)$$

Denoting $Q(\infty)$ by q,

$$N_2(r) = -\alpha_n\left[\frac{a^2(R)}{3r^3} - \frac{a(R)}{r^2} + \frac{1}{r}\right] + \alpha_n\left[\frac{a^2(R)}{3R^3} - \frac{a(R)}{R^2} + \frac{1}{R}\right] -$$

$$- \frac{\pi\alpha_n}{3}k_n + O(k_n^2 \ln k_n). \qquad (33)$$

Here $a(R) = \lim_{k_n \to 0} \delta(R)/k_n$.

Directing in (29) $r \to \infty$, we shall obtain the following equation for the phase:

$$\frac{\mathrm{tg}\,\tilde{\delta}}{k_n} = -a(R) + \frac{N_2(\infty)}{1-q} = -a(R) + \alpha_n\left[\frac{a^2(R)}{3R^3} - \frac{a(R)}{R^2} + \frac{1}{R}\right]\frac{1}{1-q} -$$
$$- \frac{\pi\alpha_n}{3(1-q)}k_n + O(k_n^2 \ln k_n). \qquad (34)$$

It is evident that the true length of scattering is

$$a(\infty) = a(R) - \alpha_n\left[\frac{a^2(R)}{3R^3} - \frac{a(R)}{R^2} + \frac{1}{R}\right]\frac{1}{1-q}. \qquad (35)$$

The greater is R, i.e. the better founded the perturbation theory applied for the accounting of V_{nn}^p, the smaller is q. At $q \leqslant 1$, the two expansion temrs found coincide with the exact one [2, 9]. For $r > R$ and small k_n the function $\varphi(r)$ itself has the following form :

$$\varphi(r) = [1 - Q(r)]\left\{r - a(R) + \frac{N_2(r)}{1-Q(r)}\right\}. \qquad (36)$$

At $r < R$ we have to the same approximation

$$\varphi(r) = r - a(R) = r - \frac{P_2(R)}{1 + P_1(R)} + O(k^2). \qquad (37)$$

Here

$$P_h(R) = \int_0^R s^k \mathcal{V}_{nn}(s)\, ds. \qquad (38)$$

Let us now consider the scattering and excitation cross section.

$$\sigma_1 = 4\pi|q_1|^2 = \frac{4\pi}{k_1^2}\sin^2\tilde{\delta}_0 = 4\pi a(\infty) + \frac{8\pi^2\alpha_1}{3}\cdot\frac{k_1 a(\infty)}{1-q} \qquad (39)$$

Here $\mathfrak{G}_1$ is the cross section of an elastic scattering, taking into account the polarization at $k_1\alpha_1 < 1$. In order to set up the dependence of q_n on k_n we must be aware of the dependence of $f(r)$ on k_1. It was found in [4] by numerical computation of the elastic scattering of electrons by hydrogen atoms that the polarization exerts its effect on the S -phase at $k_1^2 \leqslant 0.05$. A substantially greater energy is necessary to excite the levels losely bound with the basic level, and that is why we shall neglect the polarizational corrections to the functions $f(r)$ of incident electrons. We shall then represent $f(r)$ in the form of the series

$$f(r,\, k_1) = f^{(0)}(r) + k_1{}^2 f^{(1)}(r) + \ldots \qquad (40)$$

For q_n we have

$$q_n = -e^{f_i}\Bigg\{\int_0^R [r - a(R)]\,\mathcal{V}_{n1} f^{(0)}\, dr +$$

$$+ \int_R^\infty [1 - Q(r)]\left[r - a(R) + \frac{\alpha_n A(rR)}{1 - Q(r)}\right]\mathcal{V}_{n1} f^{(0)}\, dr +$$

$$+ \int_R^\infty \left[-\frac{\pi\alpha_n k_n}{3}\right]\mathcal{V}_{n1} f^{(0)}\, dr + O(k_n \ln k_n)\Bigg\} \qquad (41)$$

(we have denoted $\dfrac{a^2}{3R^3} - \dfrac{a}{R^2} + \dfrac{1}{R} - \dfrac{a^2}{3r^3} + \dfrac{a}{r^2} - \dfrac{1}{r}$ by $A(rR)$). Designating further the sum of the two first integrals by b_1, and the third by b_2, we shall obtain

$$q_n = -e^{f_i}\left[b_1 + \frac{\pi\alpha_n k_n}{3}\, b_2 + O(k_n \ln k_n)\right], \qquad (41a)$$

$$\sigma_n = 4\pi\frac{k_n}{k_1}|q_n|^2 = 4\pi\frac{k_n}{k_1}b_1{}^2\left[1 + \frac{2\pi\alpha_n b_2}{3b_1}\,k_n + O(k_n \ln k_n)\right]. \qquad (42)$$

In the same loose coupling approximation but without taking into account the polarization, the following takes place :

$$\sigma_n = 4\pi\frac{k_n}{k_1}a_1^2[1 + a_2 k_n^2] \quad [10].$$

Thus the polarization of the atom exerts a substantial effect on scattering and excitation amplitudes at low energies of incident and inelastically scattered particles respectively.

It follows from the computations of reference [4] for elastic collisions e — H, that when the energy of particles approaches the threshold of a new channel, the main role begins to be played not only by the tight coupling of the open channel with the closed ones (this coupling is taken into account by the additive polarization potential in the form (10)), but also by the virtual interaction between closed channels. Hence it follows that the polarization potential in this energy region must be nonadditive. That is why the equation (7) for elastic scattering must lead to good results only at energies below the threshold, while in prethreshold energy region it is necessary to make use of the tight bond approximation. No detailed investigations relative to excitation amplitude were conducted.

**** THE END ****

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